

Day 2: Data structures and databases

ME414: Introduction to Data Science and Big Data Analytics

LSE Methods Summer Programme

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Day 2 Outline

Data types and structures

Dataset manipulation

Compression

Relational databases and SQL

Data bases

- Relational data bases

- Normal forms

Data types and structures

What is “data science”?

- ▶ extraction or generation of knowledge from data
- ▶ extends “data mining”, using computational and algorithmic methods
- ▶ combines applied statistical methods with advances in computer science, especially machine learning
- ▶ may involve “unstructured” data, especially text, but also video and images
- ▶ closely tied to computational methods

Why focus on data types and structures?

- ▶ "data" mining and "data" science imply that we know how to work with data
- ▶ data structures are not neutral - they shape how we record, see, and have the ability to analyze information
- ▶ much of the actual work in data mining and data analysis is done at the data "munging" stage

Basic (atomic) data types in R

`numeric` 8-byte numeric representations

`integer` non-floating point numbers

`character` text

`logical` TRUE or FALSE

Recursive types also exist, such as lists and vectors; there are also special classifications for NA

Basic data types in R: integer

```
> x <- 10
> typeof(x)
[1] "double"
> is.integer(x)
[1] FALSE
> x <- 7L           # force integer type
> typeof(x)
[1] "integer"
> object.size(x)
48 bytes
> as.integer(3.14)
[1] 3
```

Basic data types in R: character

```
> typeof("test string")
```

```
[1] "character"
```

```
> object.size("a")
```

```
96 bytes
```

```
> s <- "âĈĥ" # Unicode
```

```
> cat(s)
```

```
âĈĥ
```

```
> as.character("3.14") # coerce numerics to character
```

```
[1] "3.14"
```


Basic data types in R: numeric

```
> x <- 10.5      # assign a numeric value
> x              # print the value of x

[1] 10.5

> typeof(x)      # print the class name of x

[1] "double"

> object.size(x) # show storage size in bytes

48 bytes
```

is.*() and as.*()

```
> is.numeric(x)      # is the object of numeric type?
```

```
[1] TRUE
```

```
> is.numeric(7.1)
```

```
[1] TRUE
```

```
> is.numeric("7.1")
```

```
[1] FALSE
```

```
> is.numeric(as.numeric("7.1"))
```

```
[1] TRUE
```

Basic data types in R: logical

A logical value is 'TRUE' or 'FALSE', often created via comparison between variables.

```
> 1 < 2                # is 1 less 2
```

```
[1] TRUE
```

```
> x <- c(1, 2, 3)
```

```
> y <- c(4, 3, 2)
```

```
> x > y                # vectorized comparison
```

```
[1] FALSE FALSE  TRUE
```

```
> typeof(x > y)
```

```
[1] "logical"
```

Difference between 'mode' and 'class'

- ▶ 'atomic' modes are numeric, complex, character and logical
- ▶ recursive objects have modes such as 'list' or 'function' or a few others
- ▶ an object has one and only one mode
- ▶ 'class' is a property assigned to an object that determines how generic functions operate with it - not a mutually exclusive classification
- ▶ an object has no specific class assigned to it, such as a simple numeric vector, it's class is usually the same as its mode, by convention
- ▶ an object's mode can be changed through coercion, without necessarily changing the class

Numerical precision issues

- ▶ floating point numbers are approximations of numbers
 - ▶ precision: anything more than 16 base-10 digits must be approximated
 - ▶ fractions: approximated if not $\frac{x}{2^k}$
 - ▶ anything over stated precision is truncated: $3.57\text{e}21 + 1 = 3.57\text{e}21$
 $> 1 - 4/5 - 1/5$ # *not zero!*
[1] -5.551115e-17

Machine limits

```
> .Machine$integer.max
```

```
[1] 2147483647
```

```
> .Machine[c("double.xmin", "double.xmax", "double.digits")]
```

```
$double.xmin
```

```
[1] 2.225074e-308
```

```
$double.xmax
```

```
[1] 1.797693e+308
```

```
$double.digits
```

```
[1] 53
```

Alternatives (Stata)

- ▶ single and double precision:
<http://blog.stata.com/2012/04/02/the-penultimate-guide-to-precision/>
- ▶ R has only double precision

Common input formats

- ▶ csv
- ▶ Excel
- ▶ "fixed formats"
- ▶ relational databases
- ▶ embedded tags: Extensible Markup Language (XML)
- ▶ key-value pair schemes (JSON)
 - ▶ examples of JSON and XML: <http://json.org/example>

Special issue: text encoding

- ▶ a “character set” is a list of character with associated numerical representations
- ▶ ASCII: the original character set, uses just 7 bits (2^7) – see http://ergoemacs.org/emacs/unicode_basics.html
- ▶ ASCII was later extended, e.g. ISO-8859 <http://www.ic.unicamp.br/~stolfi/EXPORT/www/ISO-8859-1-Encoding.html>, using 8 bits (2^8)
- ▶ but this became a jungle, with no standards:
http://en.wikipedia.org/wiki/Character_encoding

Solution: Unicode

- ▶ Unicode was developed to provide a unique number (a "code point") to every known character – even some that are "unknown"
- ▶ problem: there are more far code points than fit into 8-bit encodings. Hence there are multiple ways to *encode* the Unicode code points
- ▶ *variable-byte* encodings use multiple bytes as needed. Advantage is efficiency, since most ASCII and simple extended character sets can use just one byte, and these were set in the Unicode standard to their ASCII and ISO-8859 equivalents
- ▶ two most common are **UTF-8** and **UTF-16**, using 8 and 16 bits respectively

Warnings with text encodings

- ▶ Input texts can be very different
- ▶ Many text production software (e.g. MS Office-based products) still tend to use proprietary formats, such as Windows-1252
- ▶ Windows tends to use UTF-16, while Mac and other Unix-based platforms use UTF-8
- ▶ Your eyes can be deceiving: a client may display gibberish but the encoding might still be as intended
- ▶ No easy method of detecting encodings (except in HTML meta-data)

Dataset manipulation

What is a “Dataset”?

- ▶ A dataset is a “rectangular” formatted table of data in which all the values of the same variable must be in a single column
- ▶ Many of the datasets we use have been artificially reshaped in order to fulfill this criterion of rectangularity

Revisting basic data concepts

- ▶ The difference between tables and *datasets*
- ▶ This is a (partial) **dataset**:

district	incumbf	wonseatf	
1	Carlow	Kilkenny	Challenger Lost
2	Carlow	Kilkenny	Challenger Lost
5	Carlow	Kilkenny	Incumbent Won
100	Donegal	South West	Challenger Lost
459		Wicklow	Incumbent Won
464		Wicklow	Challenger Lost

- ▶ This is a **table**:

	Lost	Won
Challenger	266	60
Incumbent	32	106

- ▶ The key with a dataset is that **all the values of the same variable must be in a single column**

Example: Comparative Manifesto Project dataset

Note: Available from <https://manifestoproject.wzb.eu/>

```
> # load in a subset of the Manifesto Project dataset, with coun  
> load(url("http://kenbenoit.net/files/cmpdata.Rdata"))  
> # View(cmpdata)
```

Example: Comparative Manifesto Project dataset

This is “wide” format:

	country	countryname	oecdmember	eumember	edate	date	party	partyname
203	42	Austria	10	10	2008-09-28	200809	42320	SPOE Social Democratic Party
204	42	Austria	10	10	2008-09-28	200809	42110	Green Party
205	42	Austria	10	10	2008-09-28	200809	42520	OVP: People's Party
206	42	Austria	10	10	2008-09-28	200809	42420	FPO: Freedom Party
207	42	Austria	10	10	2008-09-28	200809	42710	BZO Alliance for the Future of Austria
208	42	Austria	10	10	2008-09-28	200809	42220	KP<d6> Communist Party of Austria
314	21	Belgium	10	10	1991-11-24	199111	21521	CVP Christian People's Party
315	21	Belgium	10	10	1991-11-24	199111	21111	ECOLO Francophone Ecologists
316	21	Belgium	10	10	1991-11-24	199111	21321	SP Flemish Socialist Party
317	21	Belgium	10	10	1991-11-24	199111	21522	PSC Christian Social Party
318	21	Belgium	10	10	1991-11-24	199111	21421	PVV Party of Liberty and Progress
319	21	Belgium	10	10	1991-11-24	199111	21913	VU People's Union
320	21	Belgium	10	10	1991-11-24	199111	21912	FDF Francophone Democratic Front

Long v. wide formats

- ▶ reshape
 - ▶ the “old” R way to do this, using ‘base::reshape()’
 - ▶ problem: confusing and difficult to use
- ▶ reshape2
 - ▶ from Hadley Wickham’s reshape2 package
 - ▶ data is first ‘melt’ed into long format
 - ▶ then ‘cast’ into desired format

Example: wide to long using reshape2

```
> require(reshape2, quietly = TRUE)
> # this will select only the "per" variables for measurement
> cmpdataLong <- melt(cmpdata,
+                      id.vars = c("countryname", "party", "date"
+                      measure.vars = names(cmpdata)[21:76],
+                      variable.name = "category",
+                      value.name = "catcount")
> # why do this?
> cmpdataLong$category <- as.character(cmpdataLong$category)
> # View(cmpdataLong)
```

Example: wide to long using reshape2

```
> require(reshape2, quietly = TRUE)
> # now we can get summary statistics across countries, e.g. for
> with(subset(cmpdataLong, grepl("^per7", category)),
+       table(countryname, category))
```

	category					
countryname	per701	per702	per703	per704	per705	per706
Austria	34	34	34	34	34	34
Belgium	63	63	63	63	63	63
Cyprus	10	10	10	10	10	10
Denmark	60	60	60	60	60	60
Finland	47	47	47	47	47	47
France	23	23	23	23	23	23
Germany	30	30	30	30	30	30
Great Britain	20	20	20	20	20	20
Greece	17	17	17	17	17	17
Iceland	31	31	31	31	31	31
Ireland	31	31	31	31	31	31
Israel	32	32	32	32	32	32
Italy	41	41	41	41	41	41
Luxembourg	21	21	21	21	21	21
Moldova	4	4	4	4	4	4

A better way

```
> require(dplyr, warn.conflicts = FALSE, quietly = TRUE)
> cmpdataLong2 <- melt(select(cmpdata, countryname, party, date,
+                             id.vars = c("countryname", "party", "date",
+                             # NOT NEEDED measure.vars = names(cmpdata
+                             variable.name = "category",
+                             value.name = "catcount")
> cmpdataLong2$category <- as.character(cmpdataLong2$category)
> identical(cmpdataLong, cmpdataLong2)

[1] TRUE
```

A better way

```
> with(filter(cmpdataLong2, grepl("^per7", category)),  
+       table(countryname, category))
```

countryname	category					
	per701	per702	per703	per704	per705	per706
Austria	34	34	34	34	34	34
Belgium	63	63	63	63	63	63
Cyprus	10	10	10	10	10	10
Denmark	60	60	60	60	60	60
Finland	47	47	47	47	47	47
France	23	23	23	23	23	23
Germany	30	30	30	30	30	30
Great Britain	20	20	20	20	20	20
Greece	17	17	17	17	17	17
Iceland	31	31	31	31	31	31
Ireland	31	31	31	31	31	31
Israel	32	32	32	32	32	32
Italy	41	41	41	41	41	41
Luxembourg	21	21	21	21	21	21
Malta	4	4	4	4	4	4
Netherlands	48	48	48	48	48	48
Norway	22	22	22	22	22	22

Grouping operations: number of parties per election

```
> # group by country-election
> by_country <- group_by(cmpdataLong, countryname, date)
> nparties <- summarise(by_country, npart = n())
> head(nparties)

# A tibble: 6 x 3
# Groups:   countryname [1]
  countryname    date npart
  <chr>    <int> <int>
1   Austria 199010   224
2   Austria 199410   280
3   Austria 199512   280
4   Austria 199910   224
5   Austria 200211   280
6   Austria 200610   280

> # is that correct?
```

Grouping operations: number of parties per election corrected

```
> # group by country-election
> by_country_unique <- distinct(cmpdataLong, countryname, date, .
> by_country_n <- group_by(by_country_unique, countryname, date)
> nparties <- summarise(by_country_n, npart = n())
> head(nparties, 10)
# A tibble: 10 x 3
# Groups:   countryname [2]
  countryname  date npart
  <chr>    <int> <int>
1   Austria 199010     4
2   Austria 199410     5
3   Austria 199512     5
4   Austria 199910     4
5   Austria 200211     5
6   Austria 200610     5
7   Austria 200809     6
8   Belgium 199111    11
9   Belgium 199505    10
10  Belgium 199906     9
```

Grouping operations: number of parties per election final

```
> # using "chaining" -- no need for intermediate objects
> nparties2 <- distinct(cmpdataLong, countryname, date, party) %
+   group_by(countryname, date) %>%
+   summarise(npart = n())
> identical(nparties, nparties2)

[1] TRUE
```


Compression in general

- ▶ Seeks to economize on space by representing recurring items using patterns that represent the uncompressed data
- ▶ Common in formats for graphics and video encoding
- ▶ "Lossless" formats compress data without reducing information - examples are .zip and .gz compression
- ▶ This (and avoiding errors) is also a principle in normalized relational data forms
- ▶ Also very important for sparse matrix representations, where many of the cells are zero, but it would be very wasteful to record a double precision numeric zero for each of these non-informative cells

Compression: sparse matrix format

Compression: sparse matrix format

used because many forms of matrix are very sparse - for example, document-term matrixes

```
> require(quantda, warn.conflicts = FALSE, quietly = TRUE)
> myDfm <- dfm(inaugTexts, verbose = FALSE)
> myDfm[1:10, 1:5]
```

Document-feature matrix of: 10 documents, 5 features (2% sparse)
10 x 5 sparse Matrix of class "dfmSparse"

	features				
docs	fellow	-	citizens	of	the
1789-Washington	3	3	5	71	116
1793-Washington	1	0	1	11	13
1797-Adams	3	5	5	140	163
1801-Jefferson	7	12	7	104	130
1805-Jefferson	8	2	10	101	143
1809-Madison	1	6	1	69	104
1813-Madison	1	1	4	65	100
1817-Monroe	6	14	9	164	275
1821-Monroe	10	6	15	197	360
1825-Adams	3	11	2	245	304

Compression: sparse matrix format

used because many forms of matrix are very sparse - for example, document-term matrixes

```
> # how many cell counts are zeros
> sum(myDfm==0) / (ndoc(myDfm) * nfeature(myDfm)) * 100
[1] 91.55164
> object.size(myDfm)
1127632 bytes
> object.size(as.matrix(myDfm))
4740208 bytes
```

Sparse matrix formats

- ▶ "simple triplet" format

 - i indexes row

 - j indexes column

 - x indicates value

- ▶ "compressed sparse column" format

 - i indexes row

 - p indexes the first nonzero element in each column of the matrix

 - x indicates value

Sparse matrix format examples

```
> # create a sparse matrix  
> require(Matrix)  
> spTmatrix <- as(Matrix(c(0, 0, 1, 2, 4, 0, 3, 0, 5), nrow = 3)  
> spTmatrix
```

3 x 3 sparse Matrix of class "dgTMatrix"

```
[1,] . 2 3  
[2,] . 4 .  
[3,] 1 . 5
```

Simple triplet matrix

```
> spTmatrix
```

```
3 x 3 sparse Matrix of class "dgTMatrix"
```

```
[1,] . 2 3
```

```
[2,] . 4 .
```

```
[3,] 1 . 5
```

```
> str(spTmatrix)
```

```
Formal class 'dgTMatrix' [package "Matrix"] with 6 slots
```

```
..@ i      : int [1:5] 2 0 1 0 2
```

```
..@ j      : int [1:5] 0 1 1 2 2
```

```
..@ Dim     : int [1:2] 3 3
```

```
..@ Dimnames:List of 2
```

```
.. ..$ : NULL
```

```
.. ..$ : NULL
```

```
..@ x      : num [1:5] 1 2 4 3 5
```

```
..@ factors : list()
```

Compressed sparse column matrix

(default for 'Matrix()' – defaults to *column* rather than *row* compressed format because R uses "column major" order matrixes)

```
> spCmatrix <- as(spTmatrix, "dgCMatrix")  
> str(spCmatrix)
```

```
Formal class 'dgCMatrix' [package "Matrix"] with 6 slots  
..@ i      : int [1:5] 2 0 1 0 2  
..@ p      : int [1:4] 0 1 3 5  
..@ Dim     : int [1:2] 3 3  
..@ Dimnames:List of 2  
.. ..$ : NULL  
.. ..$ : NULL  
..@ x      : num [1:5] 1 2 4 3 5  
..@ factors : list()
```


Compressed sparse column matrix

(default for 'Matrix()' – defaults to *column* rather than *row* compressed format because R uses "column major" order matrixes)

```
> spCmatrix <- as(spTmatrix, "dgCMatrix")  
> str(spCmatrix)
```

```
Formal class 'dgCMatrix' [package "Matrix"] with 6 slots  
..@ i      : int [1:5] 2 0 1 0 2  
..@ p      : int [1:4] 0 1 3 5  
..@ Dim     : int [1:2] 3 3  
..@ Dimnames:List of 2  
.. ..$ : NULL  
.. ..$ : NULL  
..@ x      : num [1:5] 1 2 4 3 5  
..@ factors : list()
```

Transactional databases

- ▶ Transactional databases are "ACID"
 - A tomic all of a transaction is completed, or none is completed
 - C onsistent all completed transactions leave DB in a state compliant with rules
 - I solated no results are visible until transaction is completed
 - D urable completed transactions persist, even if program crashes or exits
- ▶ "SQL" – structured query language – database managers are the most common type of relational database manager. Many variations exist, including Oracle, MySQL, PostgreSQL, and SQLite
- ▶ Most of these systems use slight variations on the same syntax, i.e. SQL
- ▶ Non-SQL based alternatives exist that do not require fixed schemas, in terms of table structures, data types, etc.
- ▶ "compressed sparse column" format
 - i indexes row
 - p indexes the first nonzero element in each column of the matrix
 - x indicates value

Databases

Relational data bases

- ▶ invented by E. F. Codd at IBM in 1970
- ▶ A relational database is a collection of data organized as a set of formally defined tables
- ▶ These tables can be accessed or reassembled in many different ways without having to reorganize the underlying tables that organize the data
- ▶ RDBMS: a relational database management system. Examples include: MySQL, SQLite, PostgreSQL, Oracle. MS Access is a lite version of this too.
- ▶ The standard user and application programmer interface to a relational database is **structured query language** (SQL)

Example

- ▶ example: Database of Parties, Elections, and Governments (DPEG) relational database

```
> #SELECT c.countryName, c.countryAbbrev, p.* FROM party AS p  
> #    LEFT JOIN country AS c  
> #    ON p.countryID = c.countryID
```

- ▶ simpler example: convert CMP data into relational tables for countries, parties, elections, categories, and counts

Basic relational structures

- ▶ tables
 - ▶ also known as “relations”
 - ▶ tables define the forms of the data that are linked to other data through key relations
- ▶ keys: how tables are cross-referenced
 - ▶ primary key: an column in a table that uniquely identifies the remaining data in the table
 - ▶ foreign key: a field in a relational table that matches the primary key column of another table
 - ▶ join operations link tables in a structured query

Normal forms 1

"Normalizing" a database means creating a proper set of relations

First normal form: No Repeating Elements or Groups of Elements

```
> head(select(cmpdata, countryname, partyname, date, per108, per110))
```

	countryname	partyname	date	per108	per110
175	Austria	FPÄ Freedom Party	199010	3	
176	Austria	GA Green Alternative	199010	0	3
177	Austria	SPÄ Social Democratic Party	199010	5	
178	Austria	ÄVP People's Party	199010	8	
179	Austria	FPÄ Freedom Party	199410	1	1
180	Austria	LF Liberal Forum	199410	0	0

Here, this is violated because of the wide format of per108 and per110.

To solve this, we have to move this to long format.

Normal forms 2

Second normal form: No Partial Dependencies on a Concatenated Key

```
> head(cmpdataLong)
```

	countryname	party	date	category	catcount
1	Austria	42420	199010	per101	0
2	Austria	42110	199010	per101	0
3	Austria	42320	199010	per101	0
4	Austria	42520	199010	per101	5
5	Austria	42420	199410	per101	0
6	Austria	42421	199410	per101	0

Here, the format is still violated, because party 42420 is repeated. To solve this we need to create a party table and link to it using a foreign key.

Normal forms 3

Third normal form: No Dependencies on Non-Key Attributes. Every non-prime attribute of data in a table must be dependent on a primary key.

```
> head(cmpdataLong)
```

	countryname	party	date	category	catcount
1	Austria	42420	199010	per101	0
2	Austria	42110	199010	per101	0
3	Austria	42320	199010	per101	0
4	Austria	42520	199010	per101	5
5	Austria	42420	199410	per101	0
6	Austria	42421	199410	per101	0

Here, this is violated because election data repeats across multiple values of the category count table, when it should have its own table.

Non-relational data

- ▶ recently popularized because so much data is unstructured, and dealing with new data forms in a classic relational setting requires changing the entire schema
- ▶ non-relational systems typically define data using **key-value** pairs
- ▶ example: JSON - see <http://kenbenoit.net/files/JSONexample.json>